

# Low rank approximations for the DEPOSIT computer code.

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## Abstract

We present an efficient technique based on low-rank separated approximations for the computation of three-dimensional integrals in the computer code DEPOSIT that describes ion-atomic collision processes. Implementation of this technique decreases the total computational time by a factor of  $\sim 10^3$ . The general concept can be applied to more complicated models.

**Keywords:** Low rank approximation, 2D cross, Separated representation, Exponential sums, 3D Integration, Slater wave function, Ion-atom collisions, Electron loss

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## 1. Introduction.

The computer code DEPOSIT [1] is intended to describe ion-atomic collision processes. It allows to calculate total and multiple electron loss cross sections  $\sigma$  and  $\sigma_m$  ( $m$  is the number of ionized electrons), the deposited energies  $T(b)$ , ( $b$  is the impact parameter of the projectile ion) and ionization probabilities  $P_m(b)$ . It is based on the energy deposition model introduced by N. Bohr [2] and developed further by A. Russek and J. Meli [3], C.L. Cocke [4], and V.P. Shevelko *et al.* [5]. Theoretical development of the DEPOSIT is presented in [5, 6, 7, 8]. Examples of calculations are reported in [9, 10, 11, 12]. Detailed description of the code and user guide are given in [1].

The cross sections and ionization probabilities needed for estimation of the losses and lifetimes of fast ion beams, background pressures and pumping requirements in accelerators and storage rings are, in fact, functionals of the deposited energy  $T(b)$ , which in turn is a three-dimensional integral over the coordinate space. To calculate any of these parameters one has to compute  $T(b)$  in all points of the  $b$ -mesh.

The integral  $T(b)$  is a bottleneck of the program, and it is required to be done as fast as possible. In the previous work [1] an advanced quadrature technique was used, and the computational time has appeared to be much faster in comparison with direct usage of uniform meshes. It takes several seconds to compute one point  $T(b)$  for one atomic shell at fixed  $b$ . For complex ions, the total computation takes few hours on one processor core and is not enough fast. To overcome this issue a fully scalable parallel variant of the algorithm was proposed. Nevertheless, the computational time is still large.

In this work, we present an entirely different approach for computing  $T(b)$  in many points of the  $b$ -mesh, based on low rank approximations of matrices and tensors. The main idea

is to approximate the functions to be integrated by a sum of products of univariate functions, effectively decreasing the dimensionality of the problem. This involves active usage of numerical and analytical tools.

The definition of  $T(b)$  involves a function of two variables (the energy gain  $\Delta E$  during an ion-atomic collision) and a function of three variables (electron density in Slater-type approximation). Details and definitions are given in Section 2.1. The integral is computed in Cartesian coordinates, which are better suited for the construction of separable representation than spherical coordinates used in the original DEPOSIT code.

In Section 2.2 for a function of two variables we use the pseudo-skeleton decomposition of matrices [13, 14, 15] computed via a variant of the incomplete cross approximation algorithm [16]. We show numerically that the function in question can be well-approximated by a separable function in Section 2.5. Thus, the approximation can be computed in  $O(n)$  time, where  $n$  is the number of grid points in one dimension.

In Section 2.3 the Slater-type function of three variables is decomposed by the exponential sums approach [17, 18]. The integral is immediately reduced to a two-dimensional one of a simpler structure.

Combining these two representations we obtain in Section 2.4 an efficient algorithm with  $O(n)$  scaling, in comparison with  $O(n^3)$  complexity for direct integration over a three-dimensional mesh. The computation of  $T(b)$  on the whole  $b$ -mesh takes less than one minute and total speedup of the program is about  $\sim 10^3$  times. Illustrative examples are given in Section 2.5.

All the equations related to the physical model are written in atomic units.

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## 2. Numerical procedure

### 2.1. Statement of the problem

The deposited energy  $T(b)$  is defined as a three-dimensional integral over coordinate space centered in the projectile ion.

$$T(b) = \sum_{\gamma} \int \Delta E_{\gamma}(p) \rho_{\gamma}(r) d^3 \mathbf{r}. \quad (1)$$

The sum here is over all atomic shells denoted by  $\gamma = nl$ ,  $n$  is the *principle quantum number* and  $l$  is the *orbital quantum number*. The electron density  $\rho_{\gamma}(r)$  is taken in a Slater-type approximation

$$\rho_{\gamma}(r) = C_{\gamma} r^{\alpha_{\gamma}} e^{-2\beta_{\gamma} r} \quad (2)$$

with integer  $\alpha_{\gamma}$ , real positive  $\beta_{\gamma}$  and normalization condition

$$\int_0^{\infty} \rho_{\gamma}(r) dr = N_{\gamma}, \quad (3)$$

where  $N_{\gamma}$  is the number of electrons in a  $\gamma$ -shell. The gain of kinetic energy  $\Delta E_{\gamma}$  is a smooth finite function of parameter  $|\mathbf{p}|$  without any singularities. The impact parameter  $\mathbf{p}$  of the ion's electron is a function of  $\mathbf{b}$  and  $\mathbf{r}$ . In frame of the moving projectile the following equality holds

$$p^2 = (b - r \cos \theta)^2 + (r \cos \varphi \sin \theta)^2. \quad (4)$$

For details we refer the reader to the paper [1]. In Cartesian coordinates  $\Delta E_{\gamma}(p)$  as a function of parameter  $p$  depends only on  $x$  and  $z$  as it follows from the equation (4)

$$T_{\gamma}(b) = \iiint \Delta E_{\gamma}(x, z - b) \rho_{\gamma}(x, y, z) dx dy dz. \quad (5)$$

Thus, we need to compute the integral (5). From here and below index  $\gamma$  will be skipped for the sake of simplicity and only one shell will be considered in the following equations.

### 2.2. Low rank approximation.

Let  $F(x, y)$  be a function of two variables  $x, y$  where point  $(x, y)$  is in a certain rectangle  $[a_x, b_x] \otimes [a_y, b_y]$ . The function is said to be in the *separated form* if it can be represented as a sum of products of univariate functions:

$$F(x, y) = \sum_{\alpha=1}^r \sigma_{\alpha} u_{\alpha}(x) g_{\alpha}(y). \quad (6)$$

The minimal number  $r$  such that (6) exists will be called *separation rank*. Direct generalization of (6) to multivariate functions is referred to as canonical polyadic (CP, also known as CAN-DECOMP/PARAFAC) [19].

If the function is in the separated form, the integration is simplified a lot. Indeed,

$$\iint F(x, y) dx dy = \sum_{\alpha=1}^r \sigma_{\alpha} \int_{a_x}^{b_x} u_{\alpha}(x) dx \int_{a_y}^{b_y} g_{\alpha}(y) dy, \quad (7)$$

and the problem is reduced to the computation of one-dimensional integrals, which can be computed using fewer quadrature points than the original integral.

The discretization of one-dimensional integrals in (7) by some quadrature formula with nodes  $x_i \in [a_x, b_x]$ ,  $i = 1, \dots, n$ ,  $y_j \in [a_y, b_y]$ ,  $j = 1, \dots, m$  and weights  $w_i^{(x)}$ ,  $w_j^{(y)}$ , leads to the approximation

$$\iint F(x, y) dx dy \approx \sum_{\alpha=1}^r \sigma_{\alpha} \sum_{i=1}^n w_i^{(x)} u_{\alpha}(x_i) \sum_{j=1}^m w_j^{(y)} g_{\alpha}(y_j). \quad (8)$$

On the other hand, direct two-dimensional quadrature with separated weights in  $x$  and  $y$  can be used for the original integral:

$$\iint F(x, y) dx dy \approx \sum_{i=1}^n w_i^{(x)} \sum_{j=1}^m w_j^{(y)} F(x_i, y_j). \quad (9)$$

Comparison of two representations (8) and (9) leads to the following discrete approximation problem

$$F(x_i, y_j) \approx \sum_{\alpha=1}^r \sigma_{\alpha} u_{\alpha}(x_i) g_{\alpha}(y_j), \quad (10)$$

which is a discrete analogue of (6). Equation (10) can be written in the matrix form:

$$A \approx U \Sigma G^T, \quad (11)$$

where  $A$  is an  $n \times m$  matrix with elements  $A_{ij} = F(x_i, y_j)$ ,  $U$  is an  $n \times r$  matrix with elements  $U_{i\alpha} = u_{\alpha}(x_i)$ ,  $G$  is an  $m \times r$  matrix with elements  $G_{j\alpha} = g_{\alpha}(y_j)$  and  $\Sigma$  is an  $r \times r$  diagonal matrix with elements  $\sigma_{\alpha}$  on the diagonal. This is a standard *low-rank approximation problem* for a given matrix. Provided that a good low-rank approximation exists, there are very efficient *cross approximation algorithms* [16, 20] that need only  $O((n + m)r)$  elements of a matrix to be computed.

By using of our implementation of the cross approximation algorithm we decompose the energy gain  $\Delta E(x, z)$  in the form (10). In Table 1 the ranks  $r$  and other numerical parameters are given for particular systems. Description of these parameters can be found in Section 2.5.

### 2.3. Exponential sums.

For a function  $\rho(x, y, z)$  defined in (2) the separation of variables can be done analytically [17, 21, 22, 18]. The main idea is to approximate the Slater density function by a sum of Gaussians

$$\rho(r) \approx \sum_{k=0}^K \lambda_k e^{-\eta_k r^2}, \quad r = \sqrt{x^2 + y^2 + z^2}. \quad (12)$$

Once the approximation (12) is computed, the separation of variables in Cartesian coordinates comes for free

$$\rho(x, y, z) \approx \sum_{k=0}^K \lambda_k e^{-\eta_k x^2} e^{-\eta_k y^2} e^{-\eta_k z^2}. \quad (13)$$

The technique for the computation of the nodes  $\lambda_k$  and the weights  $\eta_k$  is based on the computation of the inverse Laplace transform.

Table 1: Ranks  $r$  of the decomposition (32) calculated by the incomplete cross approximation algorithm [16] for the energy gain  $\Delta E(x, \bar{z})$ . Two cases are considered: collision of  $Au^{26+}$  ions with the Oxygen atom at a collision energy  $E = 6.5$  MeV/u and collision of  $U^{28+}$  ions with the Xenon atom at a collision energy  $E = 2.5$  MeV/u. Number of the  $x$ -mesh points is taken equal to  $2N + 1$ , number of the  $\bar{z}$ -mesh points is taken equal to  $3N + 1$  in correspondence to the equations (26) and (30),  $a_x = a_z = 8$ . Accuracy  $\varepsilon$  means relative error of the approximation in the Frobenius norm. The calculations were carried out on 1.3 GHz Intel Core i5 processor. Column  $T_{\text{cross}}$  corresponds to the time the cross algorithm takes. The numerical results confirm the almost linear scaling of the approach in  $N$ .

System	$\gamma$ -Shell	$r$	$T_{\text{cross}}$ (sec)	$\varepsilon$	$N$	$r$	$T_{\text{cross}}$ (sec)	$\varepsilon$	$N$	$r$	$T_{\text{cross}}$ (sec)	$\varepsilon$	$N$
$Au^{26+} + O$	$4df^{17}$	13	0.21	$10^{-6}$	1024	21	0.42	$10^{-9}$	1024	24	2.41	$10^{-9}$	4096
	$4sp^8$	13	0.21			21	0.33			24	2.40		
	$3d^{10}$	14	0.19			22	0.42			26	2.58		
	$3sp^8$	16	0.25			24	0.54			29	2.64		
	$2sp^8$	17	0.28			25	0.56			30	2.71		
	$1sp^2$	17	0.27			25	0.56			30	2.70		
$U^{28+} + Xe$	$5sp^4$	14	0.20	$10^{-6}$	1024	22	0.50	$10^{-9}$	1024	26	2.17	$10^{-9}$	4096
	$4df^{24}$	15	0.23			24	0.52			27	2.58		
	$4sp^8$	17	0.28			25	0.55			30	2.69		
	$3d^{10}$	17	0.27			25	0.54			30	2.77		
	$3sp^8$	17	0.27			25	0.55			30	2.75		
	$2sp^8$	17	0.26			25	0.54			30	2.71		
	$1sp^2$	17	0.26			25	0.55			30	2.69		

Let us consider a function  $f_{\alpha\beta}(t)$  such that its Laplace transform is function  $F_{\alpha\beta}(s)$

$$F_{\alpha\beta}(s) = \int_0^\infty e^{-st} f_{\alpha\beta}(t) dt, \quad (14)$$

of the following form:

$$F_{\alpha\beta}(s) \equiv \frac{\rho(\sqrt{s})}{C} = (\sqrt{s})^\alpha e^{-2\beta\sqrt{s}} \quad (15)$$

where  $\alpha$  and  $\beta$  are parameters of the Slater density (2). The inverse Laplace transform  $f_{\alpha\beta}(x)$  can be computed analytically for the known  $F_{\alpha\beta}(s)$ . In Appendix A we present explicit expressions for the functions  $f_{\alpha\beta}(t)$  corresponding to the functions (14) for integer  $\alpha$  and real positive  $\beta$ .

Once (14) is given and the function  $f_{\alpha\beta}(t)$  is known, the integral (14) is approximated by a quadrature formula

$$\rho(r) \approx C \sum_{k=0}^K w_k e^{t_k} f_{\alpha\beta}(e^{t_k}) e^{-r^2 e^{t_k}}, \quad (16)$$

where  $w_k$  and  $t_k$  are quadrature weights and nodes, respectively. The procedure to compute the weights and the nodes was taken from the paper [18]. For the reader's convenience we give the formula and its derivation in Appendix B.

According to equation (12)

$$\lambda_k = C w_k e^{t_k} f_{\alpha\beta}(e^{t_k}), \quad \eta_k = e^{t_k}. \quad (17)$$

It appears that only several quadrature points (at fixed  $r$ ) are required to achieve the accuracy of the expansion of order  $10^{-7}$ .

#### 2.4. Fast computation of $T(b)$ .

The three-dimensional integral  $T(b)$  defined in (5) can be reduced to a two-dimensional integral by means of the decomposition (13)

$$T(b) = \sum_{k=0}^K \lambda_k \iint \Delta E(x, z - b) e^{-\eta_k x^2} e^{-\eta_k y^2} e^{-\eta_k z^2} dx dy dz \quad (18)$$

and analytical evaluation of the one-dimensional Gaussian integral

$$\int_{-\infty}^\infty e^{-\eta y^2} dy = \sqrt{\frac{\pi}{\eta}}, \quad (19)$$

$$T(b) = \sqrt{\pi} \sum_{k=0}^K \frac{\lambda_k}{\sqrt{\eta_k}} \iint \Delta E(x, z - b) e^{-\eta_k x^2} e^{-\eta_k z^2} dx dz. \quad (20)$$

Suppose that  $\Delta E(x, z - b)$  has been decomposed as follows

$$\Delta E(x, z - b) \approx \sum_{\alpha=1}^r \sigma_\alpha u_\alpha(x) g_\alpha(z - b). \quad (21)$$

Then the integration (20) can be reduced to a sequence of one-dimensional integrations.

$$T(b) = \sqrt{\pi} \sum_{k=0}^K \frac{\lambda_k}{\sqrt{\eta_k}} \sum_{\alpha=1}^r \sigma_\alpha I_{\alpha k} J_{\alpha k}(b), \quad (22)$$

$$I_{\alpha k} = \int_{a_x}^{b_x} u_\alpha(x) e^{-\eta_k x^2} dx, \quad (23)$$

$$J_{\alpha k}(b) = \int_{a_y}^{b_y} g_\alpha(z - b) e^{-\eta_k z^2} dz. \quad (24)$$

For the numerical approximation of the integrals (23) and (24) we use the quadrature formula with uniform quadrature nodes (although any suitable quadrature can be used)

$$I_{\alpha k} = \sum_i w_i^{(x)} u_\alpha(x_i) e^{-\eta_k x_i^2}, \quad (25)$$

$$x_i = -a_x + i h_x, \quad 0 \leq i \leq 2N_x, \quad h_x = a_x/N_x, \quad (26)$$

$$J_{\alpha k}(b) = \sum_j w_j^{(z)} g_\alpha(z_j - b) e^{-\eta_k z_j^2}, \quad (27)$$

$$z_j = -a_z + j h_z, \quad 0 \leq j \leq 2N_z, \quad h_z = a_z/N_z. \quad (28)$$

We sample the impact parameter  $b$  (which can take only positive values) with the *same step*  $h_z$

$$b_l = l h_z, \quad 0 \leq l \leq N_z. \quad (29)$$

This allows us to introduce a new variable  $\tilde{z} = z - b$  discretized as

$$\tilde{z}_k = -2a_z + k h_z, \quad 0 \leq k \leq 3N_z, \quad (30)$$

and such that for the boundary conditions (28), (29), (30)

$$z_j - b_l = \tilde{z}_{j-l+N_z}. \quad (31)$$

The approximation problem (21) reduces to a low-rank approximation of the extended  $(2N_x + 1) \times (3N_z + 1)$  matrix

$$\Delta E(x_i, \tilde{z}_j) \approx \sum_{\alpha=1}^r \sigma_{\alpha} u_{\alpha}(x_i) g_{\alpha}(\tilde{z}_j). \quad (32)$$

This should be done only once (using the cross approximation algorithm), and the final approximation of the integral (27) reads

$$J_{\alpha k}(b_l) \approx \sum_j w_j^{(z)} g_{\alpha}(\tilde{z}_{j-l+N_z}) e^{-\eta_k \tilde{z}_j^2}. \quad (33)$$

The calculation of  $T(b)$  can be summarized in the following algorithm.

- 1: **for** every  $\gamma$ -shell of the projectile ion **do**
- 2:   compute the decomposition (12) for  $\rho(r)$
- 3:   compute the cross approximation for the matrix  $\Delta E(x_i, \tilde{z}_j)$  defined in (32)
- 4:   **for**  $k = 0 \dots K$  **do**
- 5:     **for**  $\alpha = 1 \dots r$  **do**
- 6:       compute the integral  $I_{\alpha k}$  defined in (25)
- 7:     **for** every  $b_l$  required **do**
- 8:       **for**  $k = 0 \dots K$  **do**
- 9:         **for**  $\alpha = 1 \dots r$  **do**
- 10:          compute the integral  $J_{\alpha k}(b_l)$  defined in (33)
- 11:       compute  $T_{\gamma}(b_l)$ , equation (22)

### 2.5. Numerical experiments.

The most important parameter in (32) is the rank  $r$ . It determines the complexity of the algorithm (the smaller  $r$ , the better). In Table 1 we present the ranks (and other numerical parameters) calculated for the energy gain  $\Delta E(x, \tilde{z})$  corresponding to different ion-atomic collisions. As it follows from the numerical experiments, the ranks are small. It means that the cross decomposition allows to decrease the size of the problem from  $O(n^2)$  elements to  $O(r \cdot n)$  elements where  $r \ll n$ .

In Table 2 we present the program speedup for every atomic shell. Details are given in the caption of the table. In sums (25) and (33) the terms less than  $\epsilon = 10^{-20}$  were thrown out for every  $x_i$  and  $\tilde{z}_j$ . It is readily seen, that the use of the technique based on the separated representations (22) allows to decrease the total time to compute  $T(b)$  by a factor of  $\sim 10^3$  compared to the previous version. In practice the computational time is reduced from several hours to one minute or less on the same hardware.

Table 2: Timings to compute  $T(b)$  at fixed  $b$  are presented for two cases: the DEPOSIT code (old)  $T_D$  and the code based on the separated representations (22)  $T_s$ . Collision systems are the same as in Table 1. Number of terms in the expansion (13) is labeled by  $N_w$ . The calculations were carried out for accuracy  $\epsilon = 10^{-7}$  and  $[-8, 8] \otimes [-16, 8]$  mesh with  $4097 \times 6145$  points. The last column shows the speedup of the program.

System	$\gamma$ -Shell	$N_w$	$T_s (\times 10^{-3} \text{ sec})$	$T_D (\text{sec})$	$T_D/T_s$
$Au^{26+} + O$	$4df^{17}$	74	7.94	3.89	490
	$4sp^8$	69	4.92	3.83	778
	$3d^{10}$	73	3.59	3.88	1080
	$3sp^8$	72	3.81	3.82	1003
	$2sp^8$	107	2.42	3.86	1592
	$1sp^2$	209	1.24	3.88	3120
$U^{28+} + Xe$	$5sp^4$	62	10.1	3.94	390
	$4df^{24}$	70	6.05	3.90	644
	$4sp^8$	67	5.00	3.94	788
	$3d^{10}$	71	3.88	3.92	1011
	$3sp^8$	70	3.52	3.90	1106
	$2sp^8$	105	1.99	3.87	1945
	$1sp^2$	207	1.04	3.88	3723

### 3. Conclusions and future work

We proposed a new technique for the computation of three-dimensional integrals based on low-rank and separated representation, that significantly reduces the computational time. The general concept can be applied to more complicated models (like ion-molecular collisions with electron loss and charge-changing processes) that lead to multidimensional integrals. For the multidimensional case we plan to use the fast approximation techniques based on the tensor train (TT) format [23].

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### Appendix A. Inverse Laplace transform sources

For integer  $\alpha$  and real positive  $\beta$  the inverse Laplace transform  $f_{\alpha\beta}(t)$  of  $F_{\alpha\beta}(s)$  from equation (14) may be calculated analytically and expressed via the *Kummer's confluent hypergeometric function*  $M(a, b; z)$  ([24], chapter 13) as follows

$$f_{\alpha\beta}(t) = \frac{M\left(1 + \frac{\alpha}{2}, \frac{1}{2}, -\frac{\beta^2}{t}\right)}{t^{1+\frac{\alpha}{2}} \Gamma\left(-\frac{\alpha}{2}\right)} - 2\beta \frac{M\left(\frac{3+\alpha}{2}, \frac{3}{2}, -\frac{\beta^2}{t}\right)}{t^{\frac{3+\alpha}{2}} \Gamma\left(-\frac{1+\alpha}{2}\right)}, \quad (A.1)$$

where

$$M(a, b; z) = 1 + \frac{a}{b} \frac{z}{1!} + \frac{a(a+1)}{b(b+1)} \frac{z^2}{2!} + \dots \quad (A.2)$$

and  $\Gamma(x)$  is the *Gamma function*.

Below we present the most interesting  $f_{\alpha\beta}(t)$  explicitly. Due to the difference of the normalization conditions in spherical and Cartesian coordinates for the Slater density (2)

$$\rho(r) = N_{\gamma} \frac{(2\beta)^{2\mu+1}}{\Gamma(2\mu+1)} r^{2\mu} e^{-2\beta r}, \quad (A.3)$$

the parameter  $\alpha$  is related to the parameter  $\mu$  as follows

$$\alpha = 2\mu - 2. \quad (\text{A.4})$$

The number of electrons in the shell  $\gamma$  is labeled as  $N_\gamma$ . The parameter  $\mu$  is greater or equal to unity. It is an integer or half-integer depending on the principal quantum number  $n$  and the orbital quantum number  $l$  of the atomic shell. Details can be found in [25, 26]. For example,  $\mu_{1s^2} = 1$ ,  $\alpha = 0$ ;  $\mu_{2sp^8} = 2$ ,  $\alpha = 2$ ;  $\mu_{4d^{10}} = 3.5$ ,  $\alpha = 5$ . Finally,

$$\begin{aligned} f_{0\beta}(t) &= \frac{g_0(t/\beta^2)}{\sqrt{\pi}\beta^2}, & g_0(t) &= \frac{e^{-\frac{1}{t}}}{t^{3/2}} \\ f_{1\beta}(t) &= \frac{g_1(t/\beta^2)}{2\sqrt{\pi}\beta^3}, & g_1(t) &= -\frac{e^{-\frac{1}{t}}}{t^{3/2}} \left(1 - \frac{2}{t}\right) \\ f_{2\beta}(t) &= \frac{3g_2(t/\beta^2)}{2\sqrt{\pi}\beta^4}, & g_2(t) &= -\frac{e^{-\frac{1}{t}}}{t^{5/2}} \left(1 - \frac{2}{3t}\right) \\ f_{3\beta}(t) &= \frac{3g_3(t/\beta^2)}{4\sqrt{\pi}\beta^5}, & g_3(t) &= \frac{e^{-\frac{1}{t}}}{t^{5/2}} \left(1 - \frac{4}{t} + \frac{4}{3t^2}\right) \\ f_{4\beta}(t) &= \frac{15g_4(t/\beta^2)}{4\sqrt{\pi}\beta^6}, & g_4(t) &= \frac{e^{-\frac{1}{t}}}{t^{7/2}} \left(1 - \frac{4}{3t} + \frac{4}{15t^2}\right) \\ f_{5\beta}(t) &= \frac{15g_5(t/\beta^2)}{8\sqrt{\pi}\beta^7}, & g_5(t) &= -\frac{e^{-\frac{1}{t}}}{t^{7/2}} \left(1 - \frac{6}{t} + \frac{4}{t^2} - \frac{8}{15t^3}\right) \\ f_{6\beta}(t) &= \frac{105g_6(t/\beta^2)}{8\sqrt{\pi}\beta^8}, & g_6(t) &= -\frac{e^{-\frac{1}{t}}}{t^{9/2}} \left(1 - \frac{2}{t} + \frac{4}{5t^2} - \frac{8}{105t^3}\right) \end{aligned}$$

## Appendix B. Quadrature formula for the Laplace integral

To obtain the decomposition (12) for given  $\alpha$  and  $\beta$  we make a substitution  $s \rightarrow s^2$  into the equation (15)

$$F_{\alpha\beta}(s^2) = s^\alpha e^{-2\beta s} = \int_0^\infty e^{-s^2 x} f_{\alpha\beta}(x) dx, \quad (\text{B.1})$$

then introduce another variable  $x = e^t$

$$F_{\alpha\beta}(s^2) = s^\alpha e^{-2\beta s} = \int_{-\infty}^\infty e^{-s^2 e^t + t} f_{\alpha\beta}(e^t) dt. \quad (\text{B.2})$$

Good news is that the function under the integral (B.2) has exponential decay both in the spatial and frequency domains, therefore the truncated trapezoidal (or more advanced) rule gives the optimal convergence rate. The final approximation has the form

$$F_{\alpha\beta}(s^2) \approx \sum_{k=0}^K w_k e^{t_k} f_{\alpha\beta}(e^{t_k}) e^{-s^2 e^{t_k}}, \quad (\text{B.3})$$

where parameters of the formula

$$t_k = a_t + kh_t, \quad h_t = (b_t - a_t)/K \quad (\text{B.4})$$

have to be selected in such a way that the resulting quadrature formula approximates the integral for a wide range of parameter  $s$ . Typically, the choice  $a_t \gtrsim -3$ ,  $b_t \lesssim 45$ , and  $K \sim 250$  gives good accuracy ( $\leq 10^{-7}$ ). As an example, in Table 2 the required number of terms in sum (B.3) is presented. Accurate error analysis can be found in [18].

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